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pyEGAF: Modernization of the EGAF database

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Abstract

One of the most comprehensive resources for thermal neutron-capture data is the Evaluated Gamma-ray Activation File (EGAF), containing data from prompt gamma activation analysis measurements carried out at the Budapest Research Reactor for 245 isotopes. Although these valuable datasets have been freely available for many years, the outdated and cryptic adopted format makes it difficult to utilize the data and it is not generally suitable for modern computational technologies. To help overcome these challenges, we have converted the datasets into an open standard JSON format. Additionally, we have developed a Python implementation of an open-source software package, pyEGAF, designed to interact with the JSON data structures for general purpose access, manipulation, and rapid assessment of the capture-gamma data in EGAF.

Keywords

Neutron-capture gamma-ray data; Partial gamma-ray cross sections; Python implementation.

Introduction

Neutron-induced reactions produce gamma-ray signatures useful in the application space ranging from nuclear security to basic science. Neutrons are generally born at high energies, however, as they downscatter and eventually thermalize, neutron capture becomes the most probable interaction. The thermal neutrons only carry a small amount of energy (~25.3 meV) resulting in the formation of an A+1 compound-nucleus [1] system in an excited state just above the neutron-separation energy following the capture reaction on the corresponding target nucleus of mass A. Because the compound nucleus is produced with an excitation energy generally below the threshold for further particle evaporation, the most likely decay mode is through the emission of electromagnetic radiation. The measured energies of the emitted gamma rays correspond to the recoil-corrected energy difference between initial and final states of the associated transitions. Accordingly, the observed gamma rays are characteristic signatures of the nucleus produced in the neutron-capture reaction, exemplifying its utility for interrogation applications, for example.

Unfortunately, and as is well known, many applications are limited by the lack of accurate or completely missing neutron-induced gamma-ray data in the evaluated neutron data libraries [2]. Efforts are currently underway to help reconcile and improve the gamma-ray data in the Evaluated Nuclear Data File ENDF/B-VIII.0 [3]. To aid this effort, one of the most useful resources containing the required thermal neutron-capture gamma-ray data is the Evaluated Gamma-ray Activation File (EGAF) [4,5]. The EGAF data were all measured in a consistent manner using the same experimental configuration employing the Prompt Gamma Activation Analysis (PGAA) [6,7,8] technique at the 10-MW Budapest Research Reactor [9,10,11] under the auspices of an International Atomic Energy Agency (IAEA) Coordinated Research Project led by the Lawrence Berkeley National Laboratory [4]. The original EGAF datasets are maintained by the IAEA online [12] in the outdated format used by the Evaluated Nuclear Structure Data File (ENSDF) [13]. In these proceedings, we summarize a new modernization effort [14] to convert the

ENSDF-formatted EGAF datasets to a JavaScript Object Notation (JSON) format along with the development of the recently deployed user-friendly thrid-party Python library, pyEGAF 1.0.0 [15,16], that is designed to interact with the new JSON schema. Collectively, these new initiatives greatly enhance access to the EGAF database and allow for the data to be utilized in a robust manner providing a convenient tool to help augment and improve the evaluated neutron-capture gamma-ray data according to needs and actions outlined in Ref. [2].

Modernization of the EGAF format and the pyEGAF library

The original mixed-record 80-character column ENSDF format [13] is cryptic, space-limited and difficult to work with. This dated format is representative of a much earlier era in computing and is not generally suitable for modern computational processing codes and technologies. Due to the complexity of the format, usually only very experienced users or ENSDF evaluators have the familiarity required to utilize the datasets in a meaningful way and a parser is needed to interpret the different fields in a given record. Ergo, this limits accessibility of EGAF data to small number of people, often rendering projects deficient that would otherwise benefit from the thermal neutron-capture gamma-ray data contained in the EGAF database. The format translation effort, described in detail in Ref. [14], aims to mitigate these legacy issues and also benefits from earlier work to convert ENSDF datasets into an eXtensible Markup Language (XML) format; the laboratory report in Ref. [17] describes an early implementation of the corresponding ENSDF-to-XML parser. A total of 245 ENSDF-formatted EGAF datasets have been translated into an open standard JSON format [14,15,16] enabling accessibility to applications using different programming languages running in different environments. The schematic of the partial nuclear chart in Fig. 1 shows the target nuclides and corresponding compound-nucleus residuals relevant to the EGAF project.

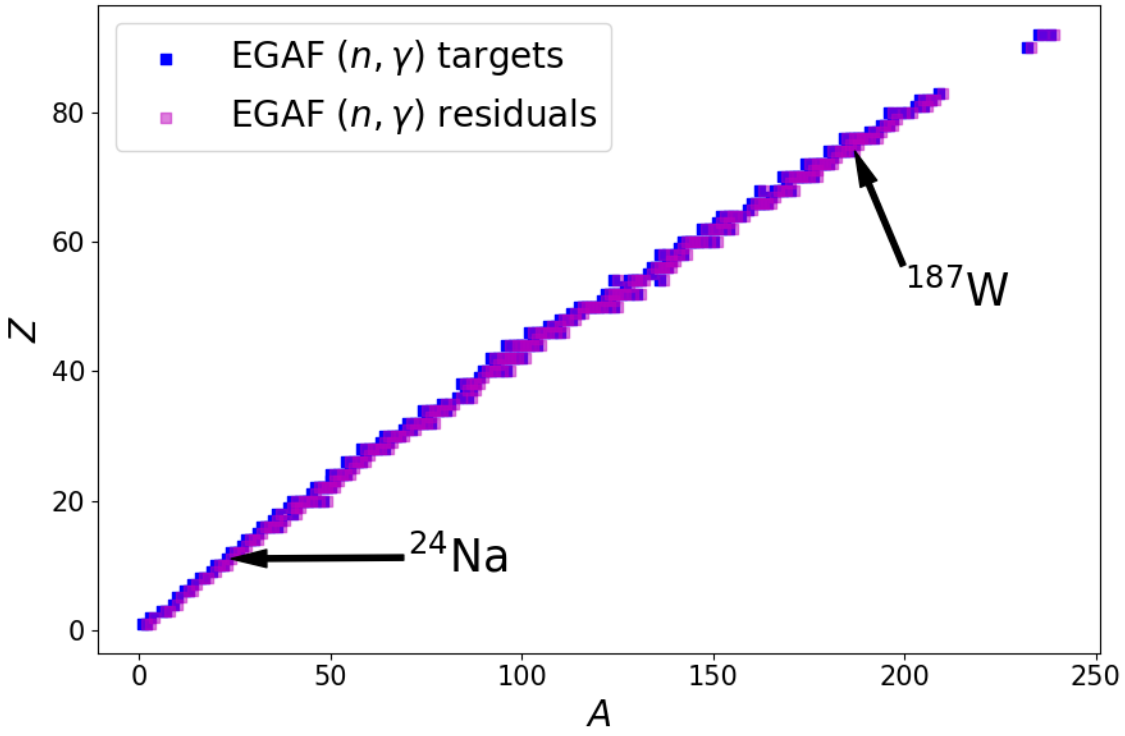

Fig.1 Partial schematic of the nuclear landscape showing the target nuclides (blue squares) and corresponding (A+1) compound-nucleus residuals (semi-transparent magenta squares) of relevance to the EGAF project. The positions of the residual nuclides ^{24}Na and ^{187}W are labeled.

The JSON data structures support data types including: *string*; *number*; *boolean*; *null*; *object* (JSON object); and *array*. All data explicitly reported in the primary and continuation records of the ENSDF file associated with the "*Level*", "*Gamma*", and "*Normalization*" record [13] have been interpreted and sourced into the JSON data structures. The principal data derived from here are the gamma-ray energies and corresponding partial gamma-ray cross sections together with nuclear structure decay-scheme properties and all associated uncertainties. Independent values of the total radiative thermal neutron capture cross sections taken from the *Atlas of Neutron Resonances* [18,19] are also provided in addition to data that is only implicit in the original EGAF files such as the level indices and final-level information associated with

93each gamma-ray transition. For a more complete description of the data included in the 94JSON data structures see Ref. [14]. An intuitive syntax has also been adopted for the 95keys of the JSON schema, explained in detail in the README documentation available 96on GitHub [15].

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98In addition to the JSON format, because many nuclear reaction codes used for modeling 99and evaluation, e.g., CoH_3 [20], EMPIRE [21], TALYS [22], and DICEBOX [23], source 100the Reference Input Parameter Library (RIPL) [24] or RIPL-like formatted datasets, we 101have also translated each of the EGAF datasets into a representative RIPL format. The 102RIPL-formatted EGAF datasets contain a subset of the information from the original 103EGAF datasets as described in Ref. [14], along with the neutron- and proton-separation 104energy values taken from the *AME2020 atomic mass evaluation* [25].

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106To improve accessibility to EGAF and better enable interaction, manipulation, analysis, 107and visualization of the neutron-capture gamma-ray data, we have also developed a 108Python implementation of an open-source software package, pyEGAF [14,15,16], 109designed for interaction with the translated JSON data structures. The software package 110consists of a suite of 9 Python modules containing several classes and functions for 111handling the capture-gamma data in EGAF. All classes and methods have supporting 112docstrings including examples illustrating known use cases for all functions. The original 113ENSDF-formatted EGAF datasets along with the translated RIPL- and JSON-formatted 114datasets are bundled together with the software; a total of 735 datasets. Additionally, a 115test suite containing more than 200 unit tests is provided. These tests are called from a 116configuration file and are automatically started after building against virtual Python 117environments. To illustrate use of pyEGAF, an overview of the methods is provided in 118the Jupyter Notebooks that also accompany the software [15]. The pyEGAF software 119package is freely distributed and licensed through the FreeBSD Documentation License. 120It is available on both GitHub [15] and through the Python Package Index (PyPI)

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repository [16]. Building, installation, running and testing details are described in the associated README [15] and DESCRIPTION [16] documentation.

Applications of pyEGAF

The neutron-capture reaction is important for both societal and basic science applications. Accordingly, pyEGAF lends itself to many applications – a few of which are discussed in Ref. [14], e.g., nuclear forensics; pyEGAF now provides the capability to conveniently search the EGAF database by gamma-ray energy and provides functionality to retrieve the strongest gamma rays in a given compound nucleus. Statistical-model related applications and nuclear structure decay-scheme data validation represent another key use of pyEGAF. The adopted methodologies in these areas will be useful in helping to address the needs and reconcile problems, e.g., missing or incomplete data, in the evaluated neutron data libraries outlined in Ref. [2]. Furthermore more, because pyEGAF allows users to retrieve and manipulate the EGAF data in a user-friendly and straightforward manner, we can now rapidly assess and visualize properties of nuclei across a particular subset, or even all nuclides in the EGAF database.

Assessment of the *primary* gamma rays, typically high-energy gamma-rays that are observed to deexcite the capture state in the region of the corresponding neutron-separation energy following thermal neutron capture, is particularly useful in material identification and nondestructive-assay applications. To this end, pyEGAF allows users to identify and examine all primary gamma rays from a given isotope or set of isotopes. Because these gamma rays are characteristic of the isotopes present in an interrogated medium, they can help pin down its isotopic composition. Additionally, pyEGAF allows users to specify their preferred intensity quantity, i.e., absolute elemental or isotopic partial gamma-ray cross sections, populations per neutron capture, or relative intensities [14]. These intensities can also be readily renormalized or incorporated into an analysis framework for simulations allowing for direct comparison with real experimental data.

Moreover, we can compare the total measured primary-gamma-ray intensity (σ_γ) to the corresponding independent adopted values [18,19] for the total thermal neutron-capture cross sections (σ_0) that are also in EGAF, to provide a measure of completeness of the primary capture-gamma spectrum:

$$f = \frac{\Sigma_{i=1} \sigma_\gamma (1+\alpha_i)}{\sigma_0} \qquad (1)$$

where α represents the internal-conversion coefficient and the summation in Eq. (1) goes over all reported primaries for a given residual nucleus in EGAF. Internal conversion is usually negligible for high-energy primaries. Provided that all statistically-significant primary gamma rays have been accounted for, the numerator in Eq. (1) also provides a measurement of the total neutron-capture cross section at thermal-incident neutron energies. Thus, cases where f=1 are suggestive of a complete primary gamma-ray spectrum, e.g., ^{23}Na(n, γ) where f=0.99(2). Often, however, only a fraction of the emitted primary gamma rays are observed leading to values of f<1, e.g., ^{186}W(n, γ) where f=0.37(1), and in such cases statistical models are needed to account for the missing component of the total decay intensity from the non-discrete neutron-capture state [26]. Fig. 2 summarizes the completeness of the primary gamma-ray spectra for the residual nuclides in the EGAF database; the f=1 nuclides generally occupy distinctly different regions of the nuclear landscape shown in Fig. 1., e.g., ^{24}Na (complete) in the lighter-*A* region and ^{187}W (incomplete) in the heavier-*A* region. However, the plot shown in Fig. 2 can help guide recommendations for new measurements where primary gamma-ray experimental data are lacking. In certain cases, we have also found values of f>1; such a situation is not physical, however, and these results have not been included in the plot. Any results with f>1 likely imply either the total neutron capture cross section is not well established, or the primary gamma-ray intensities are poorly measured. Because the EGAF measurements utilized natural samples, gamma-ray lines from some of the weaker isotopes in the element are often harder to measure unambiguously or may be swamped by stronger signals nearby leading to less accurate measurements of the corresponding gamma-ray intensity. Indeed there are many cases where this ratio fails to reach a value

176of f>0.9 and so these results can also be used to support recommendations regarding 177future experimental work for important materials serving different applications outlined 178in Ref. [2].

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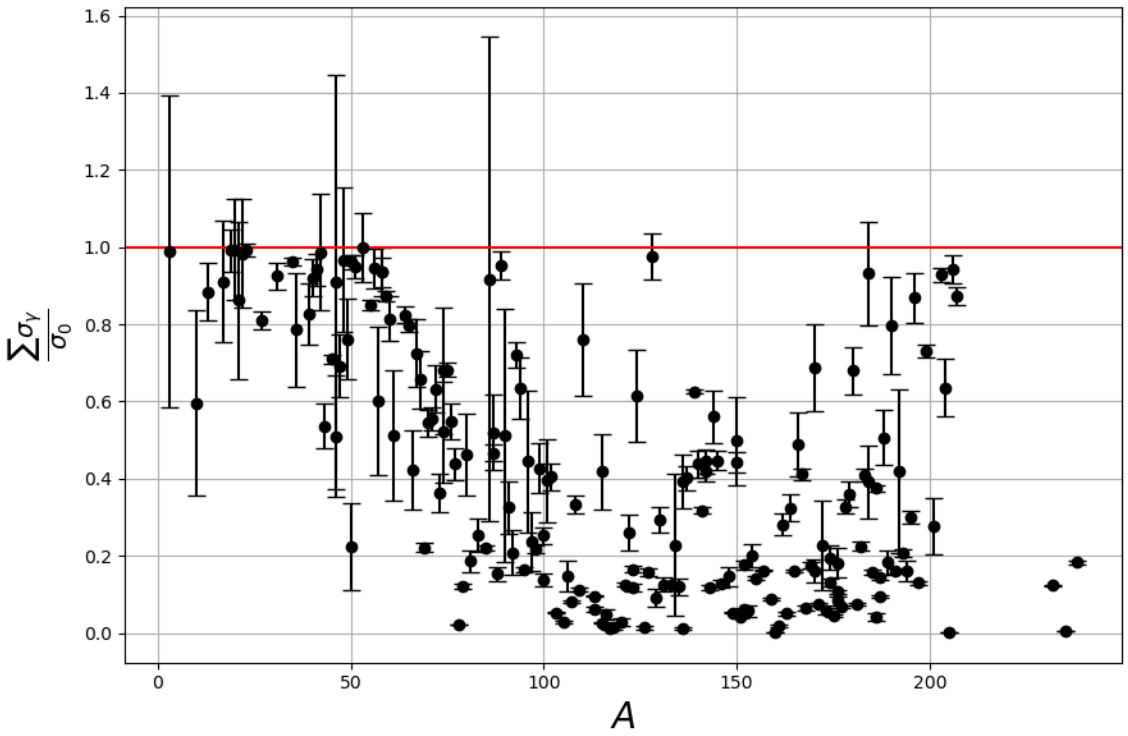

181 **Fig. 2** Ratio of the summed measured intensity of all primary gamma rays observed in
182 each A+1 compound nucleus in EGAF to the independent value of the total radiative
183 thermal neutron-capture cross section for corresponding target A nucleus taken from
184 Refs. [18,19], as appropriate. Only values where this ratio is less than or equal to 1 are
185 shown on the plot.

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187 **Summary**

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188The original EGAF database [4,5,12] has been completely modernized and translated into
189a new JSON format [14]. A representative RIPL format for each EGAF data set has also
190been generated providing a realistic set of levels and gammas for use in statistical model
191calculations to simulate the thermal (n, γ) reaction. These reformatted JSON and RIPL
192datasets are bundled together with the orginal ENSDF-formatted EGAF datasets as part
193of an open-source Python implementation of the third-party library, pyEGAF [15,16].
194The development of pyEGAF provides users with a convenient means to interact,
195manipulate, analyze, and visualize the thermal neutron-capture gamma-ray data and
196associated nuclear structure and meta data contained in the EGAF database. This
197software package is already being used as a tool to help reconcile and improve the
198neutron-capture gamma-ray data in the evaluated nuclear data libraries [2]. It is
199anticipated that future versions of the pyEGAF library will be developed to include
200additional information such as extensive sets of Band-Raman calculated internal
201conversion coefficients (BrIcc) [27], as well as updated thermal neutron-capture gamma-
202ray data based on more recent measurements involving isotopically-enriched targets, e.g.,
203the tungsten isotopes [26,28] and iron [29], in addition to newly adopted total neutron-
204capture cross-section values.

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